NumLin: Linear Types for Numerical Libraries

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Abstract. Briefly summarize the contents of the paper in 150–250 words.

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1 Introduction

Numlin is a functional programming language designed to express the APIs of low-level linear algebra libraries (such as BLAS/LAPACK) safely and explicitly. It does so by combining linear types, fractional permissions, runtime errors and recursion into a small, easily understandable, yet expressive set of core constructs. In addition to this, Numlin's implementation supports several syntactic conveniences as well as a usable integration with real-world OCaml code.

1.1 Contributions

- We have designed the NumLin programming language
- We illustrate that the design is sensible with many matrix-y examples
- We give a soundness proof for NumLin, using a step-indexed logical relation
- Incredibly simple type inference algorihtm for polymorphic fractional permissions
 - Compare to Bierhof et al's Fraction Polymorphic Permission Inference, which uses a fancy dataflow analysis
 - We use exactly the same unification algorithm type polymorphism does
- We have an implementation compatible with and usable from existing code!

2 NumLin Overview and Examples

2.1 Overview

Linearity is at the heart of NumLin. Linearity allows us to express a purefunctional API for numerical library routines that mutate arrays and matrices. Linearity also restricts aliasing of (values which represent) pointers. Intuitionism: ! and Many However, linearity by itself is not sufficient to produce an expressive enough programming language. For values such as booleans, integers, floating-point numbers as well as pure functions, we need to be able to use them *intuitionistically*, that is, more than once or not at all. For this reason, we have the ! constructor at the type level and its corresponding Many constructor and let Many <id> = . . in . . eliminator at the term level. Because we want to restrict how a programmer can alias pointers and prevent a programmer from ignoring them (a memory leak), Numlin enforces simple syntactic restrictions on which values can be wrapped up in a Many constructor (details in Section 3).

Fractional Permissions There are also valid cases in which we would want to alias pointers to a matrix. The most common is exemplified by the BLAS routine gemm, which (rather tersely) stands for $GEneric\ Matrix\ Multiplication$. A simplified definition of gemm(α , A, B, β , C) is $C := \alpha AB + \beta C$. In this case, A and B may alias each other but neither may alias C, because it is being written to. Related to mutating arrays and matrices is freeing them. Here, we would also wish to restrict aliasing so that we do not free one alias and then attempt to use another. Although linearity on its own suffices to prevent use-after-free errors when values are not aliased (a freed value is out of scope for the rest of the expression), we still need another simple, yet powerful concept to provide us with the extra expressivity of aliasing without losing any of the benefits of linearity.

Fractional permissions provide exactly this. Concretely, types of (pointers to) arrays and matrices are parameterised by a fraction. A fraction is either 1 (2^0) or exactly half of another fraction (2^{-k} , for natural k). The former represents complete ownership of that value: the programmer may mutate or free that value as they choose; the latter represents read-only access or a borrow: the programmer may read from the value but not write to or free it. Creating an array/matrix gives you ownership of it, so too does having one (with a fractional permission of 2^0) passed in as an argument.

In NumLin, we can produce two aliases of a single array/matrix, by sharing it. If the original alias had a fractional permission of 2^{-k} then the two new aliases of it will have a fractional permission of $2^{-(k+1)}$ each. Thanks to linearity, the original array/matrix with a fractional permission of 2^{-k} will be out of scope after the sharing. When an array/matrix is shared as such, we can prevent the programmer from freeing or mutating it by making the types of free and set (for mutation) require a whole (2^0) permission.

If we have two aliases to the same matrix with identical fractional permissions $(2^{-(k+1)})$, we can recombine or unshare them back into a single one, with a larger 2^{-k} permission. As before, thanks to linearity, the original two aliases will be out of scope after unsharing.

Runtime Errors Aside from out-of-bounds indexing, matrix unsharing is one of only *two* operations that can fail at runtime (the other being dimension checks,

such as for gemm). The check being performed is a simple sanity check that the two aliasing pointers passed to unshare point to the same array/matrix. Section 5 contains an overview of how we could remove the need for this by tracking pointer identities statically by augmenting the type system further.

Recursion The final feature of NumLin which makes it sufficiently expressive is recursion (and of course, conditional branches to ensure termination). Conditional branches are implemented by ensuring that both branches use the same set of linear values. A function can be recursive if it captures no linear values from its environment. Like with Many, this is enforced via simple syntactic restrictions on the definition of recursive functions.

2.2 Examples

The more examples, the better. In fact, it's actually impossible to have too many examples – it's okay (indeed, desirable) to spend 5-6 pages on examples.

- Simple: factorial, shows recursion, ! annotations etc.
- Less simple: summing over an array, indexing and safety
- Medium: one-dimensioal convolution, permissions
- Harder: linear regression, pattern-matching and apparent non-linearity
- Harder: L1 norm-minimisation, some frees, re-using memory
- Big finish: Kalman filter

Factorial Although a factorial function (Figure 1) may seem like an aggresively pedestrian first example, in a linearly typed language such as NumLin it represents the culmination of many features.

To simplify the design and implementation of NumLin's type system, recursive functions must have full type annotations (non-recursive functions need only their argument types annotated). Its body is a closed expression (with respect to the function's arguments), so it type-checks (since it does not capture any linear values from its environment).

The only argument is !x : !int. The ! annotation on x is a syntactic convenience for declaring the value to used intuitionistically, its full and precise meaning is described in Section 4.

The condition for an if may or may not use linear values (here, with $\mathbf{x} < 0$) | | $\mathbf{x} = 0$, it does not). Any linear values used by the conditional would not be in scope in either branch of the if-expression. Both branches use \mathbf{x} differently: one ignores it completely and the other uses it twice.

All numeric and boolean literals are implicitly wrapped in a Many and all primitives involving them return a !int, !bool or !elt (types of elements of arrays/matrices, typically 64-bit floating-point numbers). The short-circuting | | behaves in exactly the same way as a boolean-valued if-expression.

Fig. 1. Factorial function in NumLin.

Fig. 2. Summing over an array in NumLin.

Summing over an Array Now we can add fractional permissions to the mix: Figure 2 shows a simple, tail-recursive implementation of summing all the elements in an array. There are many new features; first among them is !x0 : !elt, the type of array/matrix elements (64-bit floating point).

Second is ('x) (row: 'x arr) which is an array with a universally-quantified fractional permission. In particular, this means the body of the function cannot mutate or free the input array, only read from it. If the programmer did try to mutate or free row, then they would get a helpful error message (Figure 3).

Alongside taking a row: 'x arr, the function also returns an array with exactly the same fractional permission as the row (which can only be row). This is necessary because of linearity: for the caller, the original array passed in as an argument would be out of scope for the rest of the expression, so it needs to be returned and then rebound to be used for the rest of the function.

An example of this consuming and re-binding is in let (row, !x1) = row[i]. Indexing is implemented as a primitive get: 'x. 'x arr --o !int --o 'x arr * !elt. Although fractional permissions can be passed around explicitly (as done in the recursive call), they can also be automatically inferred at call sites, row[i] == get _ row i takes advantage of this convenience.

One-dimensional Convolution Figure 4 extends the set of features demonstrated by the previous examples by mutating one of the input arrays. A one-dimensional convolution involves two arrays: a read-only kernel (array of weights) and an input vector. It modifies the input vector *in-place* by replacing each write[i] with a weighted (as per the values in the kernel) sum of it and its neighbours; intuitively, sliding a dot-product with the kernel across the vector.

Fig. 3. Attempting to write to or free a read only array in NumLin.

```
let rec simp_oned_conv
        (!i : !int) (!n : !int) (!x0 : !elt)
        (write : z arr) ('x) (weights : 'x arr)
        : z arr * 'x arr =
    if n = i then (write, weights) else
    let !w0 <- weights[0]</pre>
                              in
    let !w1 <- weights[1]</pre>
                              in
    let !w2 <- weights[2]</pre>
    let !x1 <- write[i]</pre>
                              in
    let !x2 <- write[i + 1] in
    let written = write[i] := w0 *. x0 +. (w1 *. x1 +. w2 *. x2) in
    simp_oned_conv (i + 1) n x1 written _ weights in
  simp_oned_conv
;;
```

 ${\bf Fig.\,4.}\ Simplified\ {\bf one-dimensional\ convolution}.$

What's implemented in Figure 4 is a *simplified* version of this idea, so as to not distract from the features of NumLin. The simplifications are:

- the kernel has a fixed length (of 3), as such, only the value of write[i-1] prior to modification in the previous iteration needs to be carried forward using x0
- write is assumed to have length n+1
- i's initial value is assumed to be 1
- x0's initial value is assumed to be write[0]
- the first and last values of write are ignored.

Mutating an array is implemented similarly to indexing one: a primitive set: z arr --o !int --o !elt --o z arr. It consumes the original array and returns a new array with the updated value. let written = write[i] := <exp> is just syntactic sugar for let written = set write i <exp>.

Since write: z arr (where z stands for k=0, representing a fractional permission of $2^{-k}=2^{-0}=1$), we may mutate it, but since we only need to read from weights, its fractional permission index can be universally-quantified. In the recursive call, we see _ being used explicitly to tell the compiler to *infer* the correct fractional permission based on the given arguments.

Fig. 5. Linear regression (OLS): $\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$

Linear Regression The most pertinent aspect of NumLin's type system are the types of its primitives. While the types of operations such as get and set might be borderline obvious, they types of BLAS/LAPACK routines become an incredibly useful, automated check for using the API correctly.

Figure 5 shows a *non-recursive* function declaration (the return type is inferred). Since we would like to be able to use a function like lin_reg more than once, it is marked with a ! annotation (which also ensure it captures no linear values from the surrounding environment).

We wish to compute $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$. First, we extract the dimensions of matrix \mathbf{x} . Then, we say we would like a new matrix, of dimension $m \times 1$, which contains the result of $\mathbf{X}^T\mathbf{y}$. The line let $\mathbf{x}\mathbf{y} < -$ new $(\mathbf{m}, 1)$ [| $\mathbf{x}^T\mathbf{x}$ \text{y} |] is syntactic sugar for first creating a new matrix let $\mathbf{x}\mathbf{y} = \mathbf{matrix} \ \mathbf{m} \ 1$ in and then storing the result of $(\mathbf{x}, \text{ true } (* \text{ transp'd } *))$ multiplied with $(\mathbf{y}, \text{ false } (* \text{ not transp'd } *))$ into $\mathbf{x}\mathbf{y}$: let $(\mathbf{x}\mathbf{y}, (\mathbf{x}, \mathbf{y})) = \mathbf{gemm} \ 1$. _ $(\mathbf{x}, \text{ true})$ _ $(\mathbf{y}, \text{ false})$ 0. $\mathbf{x}\mathbf{y}$, appropriately re-binding the identifiers. The line let $\mathbf{x}_T\mathbf{x} < -$ new (\mathbf{m},\mathbf{m}) [| $\mathbf{x}^T\mathbf{x} \mathbf{x}$ |], works similarly, but uses a more appropriate, $\mathbf{x}\mathbf{y}\mathbf{x}\mathbf{x}$ true 1. \mathbf{x} 0. $\mathbf{x}_T\mathbf{x}$ BLAS call.

By using some simple pattern-matching and syntactic sugar, we can:

- write normal-looking, apparently non-linear code
- use matrix expressions directly and have an appropriate, efficient call to a $\rm BLAS/LAPACK$ routine inserted
- retain the safety of linear types with fractional permissions by having the compiler statically enforce the aliasing and read/write rules implicitly assumed by BLAS/LAPACK routines.

After computing x_T_x, we need to invert it and then multiply it by xy. The BLAS routine posv: z mat --o z mat * z mat does exactly that: assuming the first argument is symmetric, posv mutates its second argument to contain the desired value. Its first argument is also mutated to contain the (upper triangular) Cholesky decomposition factor of the original matrix. Since we do not need that matrix (or its memory) again, we free it. If we forgot to, we would get a Variable to_del not used error. Lastly, we return the answer alongside the untouched input matrices (x,y).

```
let !11_norm_min (q : z mat) (u : z mat) =
  let (u , (!_n, !k)) = sizeM _ u in
  let (u , u_T ) = transpose _ u in
  let (tmp_n_n , q_inv_u ) = gesv q u in
  let i = eye k in
  let to_inv <- [| i + u_T * q_inv_u |] in
  let (tmp_k_k, inv_u_T ) = gesv to_inv u_T in
  let () = freeM tmp_k_k in
  let answer <- [| 0. * tmp_n_n + q_inv_u * inv_u_T |] in
  let () = freeM q_inv_u in
  let () = freeM inv_u_T in
  answer in

11_norm_min
;;</pre>
```

Fig. 6. L1-norm minimisation on manifolds: $\mathbf{Q}^{-1}\mathbf{U}(\mathbf{I} + \mathbf{U}^{T}\mathbf{Q}^{-1}\mathbf{U})^{-1}\mathbf{U}^{T}$

L1-Norm Minimisation on Manifolds Figure 6 shows even more pattern-matching. Patterns of the form let $\langle id \rangle \langle -[|beta*c+alpha*a*b|]$ are desugared to gemm calls. Primitives like transpose: 'x. 'x mat --o 'x mat * z mat and eye: !int --o z mat allocate new matrices; transpose returns the transpose of a given matrix and eye returns a $k \times k$ identity matrix.

We also see our first example of re-using memory for different matrices: like with to_del and posv in the previous example, we do not need the value stored in tmp_5_5 after the call to gesv. However, we can use the memory much later to store answer with let answer <- [| 0. * tmp_5_5 + q_inv_u * inv_u_T |]. Again, thanks to linearity, the identifiers q, tmp_5_5 are out of scope by the time answer is bound. Although during execution, all three refer to the same piece of memory, logically they represent different values throughout the computation.

Kalman Filter Figure 7 shows a NumLin implementation of a Kalman filter (equations in Figure 8). A few new features and techniques are used in this implementation:

- sym annotations in matrix expressions: when this is used, a call to symm
 (the equivalent of gemm but for symmetric matrices so that only half the
 operations are performed) is inserted (instead of one to gemm)
- copyM_to is used to re-use memory by overwriting the contents of its second argument to that of its first (erroring if dimensions do not match)
- let new_r <- new [| r_2 |] creates a copy of r_2
- potrs _ chol_r data_2 uses a pre-computed Cholesky decomposition to multiply data_2 by $r_2 = (R + H\Sigma H^T)^{-1}$
- a lot of memory re-use; the following sets of identifiers alias each other:
 - r_1 and r_2
 - data_1, data_2 and sol_data

```
let !kalman
       ('s) (sigma : 's mat) (* n, n *)
       ('h) (h : 'h mat)
                           (* k.n *)
       ('m) (mu : 'm mat)
                           (* n, 1 *)
                             (* k, k *)
       (r_1 : z mat)
                            (* k, 1 *) =
       (data_1 : z mat)
       let (h, (!k, !n)) = sizeM _ h in
(*16*) let sigma_h <- new (k, n) [| h * sym (sigma) |] in
(*17*) let r_2 <- [| sigma_h * h^T + r_1 |] in
(*18*) let data_2 <- [| h * mu - data_1 |] in
(*19*) let (h, new_h) = copyM_to _ h sigma_h in
(*20*) let new_r <- new [| r_2 |] in
(*21*) let (chol_r, sol_h) = posv new_r new_h in
(*23*) let (chol_r, sol_data) = potrs _ chol_r data_2 in
       let () = freeM (* k, k *) chol_r in
(*24*) let h_sol_h <- new (n, n) [| h^T * sol_h |] in
       let () = freeM (* k, n *) sol_h in
(*25*) let h_sol_data <- new (n, 1) [| h^T * sol_data |] in
(*26*) let mu_copy <- new [| mu |] in
(*27*) let new_mu <- [| sym (sigma) * h_sol_data + mu_copy |] in
       let () = freeM (* n, 1 *) h_sol_data in
(*28*) let h_sol_h_sigma <- new (n,n) [| h_sol_h * sym(sigma) |] in
(*29*) let (sigma, sigma_copy) = copyM_to _ sigma h_sol_h in
(*30*) let new_sigma <- [| sigma_copy - sym (sigma) * h_sol_h_sigma |] in
       let () = freeM (* n, n *) h_sol_h_sigma in
       ((sigma, (h, (mu, (r_2, sol_data)))), (new_mu, new_sigma)) in
     kalman
     ;;
```

Fig. 7. Kalman filter: see Figure 8 for the equations this code implements.

- new_h and sol_h
- h_sol_h, sigma_copy and new_sigma
- mu_copy and new_mu

3 Formal System

3.1 The Core Type Theory and Dynamic Semantics

Describe the typing rules and operational semantics here

3.2 The logical relation

Describe the step-indexed logical relation and its main properties

3.3 Soundness Theorem

State the fundamental lemma, and sketch the proof a little

$$\mu' = \mu + \Sigma H^T (R + H\Sigma H^T)^{-1} (H\mu - \text{data})$$

$$\Sigma' = \Sigma (I - H^T (R + H\Sigma H^T)^{-1} H\Sigma)$$

Fig. 8. Kalman filter equations (credit: matthewrocklin.com).

4 Implementation

4.1 Implementation Strategy

Talk about how you implemented NumLin and the general architecture. Talk about how simple everything is, and also about how implementing inference for fractions is.

4.2 Performance Metrics

Here, evaluate the performance of the examples from the second section. Compare with your C implementations, and perhaps as well as the straightforward math transcribed into (Matlab/R/Numpy?).

5 Discussion and Related Work

The main point we want to make is that using linear types for BLAS is an "obvious" idea, but is surprisingly under-explored.

- Rust
- ATS
- Single-assignment C
- Linear Haskell
- Bernardy and Sveningsson
- L3
- Boyland fractional permissions

References